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Intra- and intermolecular interactions in the series of acyclic and macrocyclic compounds containing nucleotide bases and their derivatives

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Abstract

Intra-and intermolecular interactions in acyclic compounds containing nucleotide base (uracil and thymine) derivatives and their macrocyclic analogs (pyrimidinophanes) were studied by IR, UV, luminescence, and NMR spectroscopy. Molecules of these compounds include one or two N3-methylsubstituted or N3-unsubstituted uracil fragment or two adenine fragments linked through a hexamethylene spacer to an uracil, 5,5'-methylenediuracil or diphenylmethane fragment. The examined compounds almost all are characterized by π-π interactions and intramolecular hydrogen bonding between the terminal uracil or adenine fragments. Intramolecular association constants were determined and factors affecting them were discussed. Complex formation of acyclic and macrocyclic ligands with adenine and thymine derivatives was studied. The low values of the association constants were interpreted in terms of a competition between intra-and intermolecular bonding and very labile ligand structure.

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